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ADLAYER PHYSICS

Syracuse University

Peter A. Dowden

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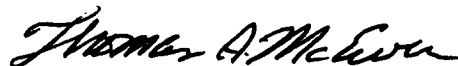
Rome Air Development Center
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<p>This report summarizes the results of a post-doctoral research effort performed at Syracuse University. The research conducted has led to an improved understanding of the physics of thin metal overlayers. Specific findings include: 1) the work function of adlayers cannot be determined by simply considering the influences of local chemistry and charge transfer due to chemical bonding; 2) long range crystallographic order has been shown to have influence on electronic structure and density of states in thin metal overlayers; 3) thin metal films can be strained by changing the lattice constant of a material, the resulting strain is proportional to the change in the valence band electron structure.</p>					
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The goals of this project were largely directed toward the relationship between the electronic structure and properties of large Z metals and the local crystallography. Of particular interest were the group II metals (Ba, Sr, Hg) in very thin films. The emphasis of this research was to characterize the correlation between electronic structure as determined by the density of states and work function with lattice constant and crystallographic order.

A variety of techniques were used in this investigation including low energy electron diffraction (LEED), angle-resolved photoemission (ARUPS), and constant initial state photoemission (CIS).

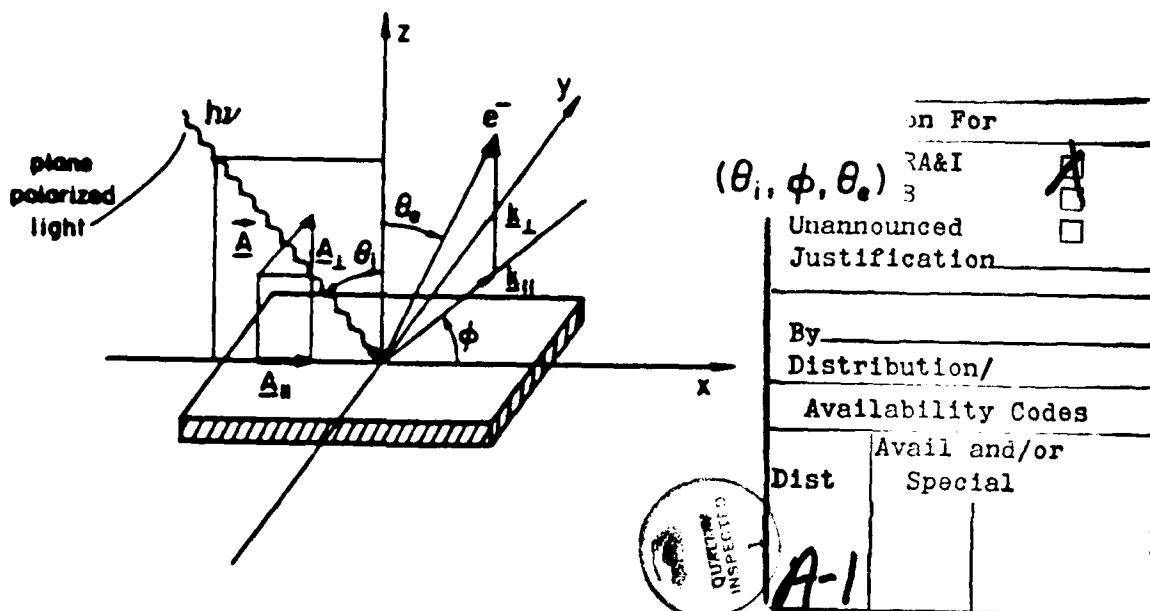
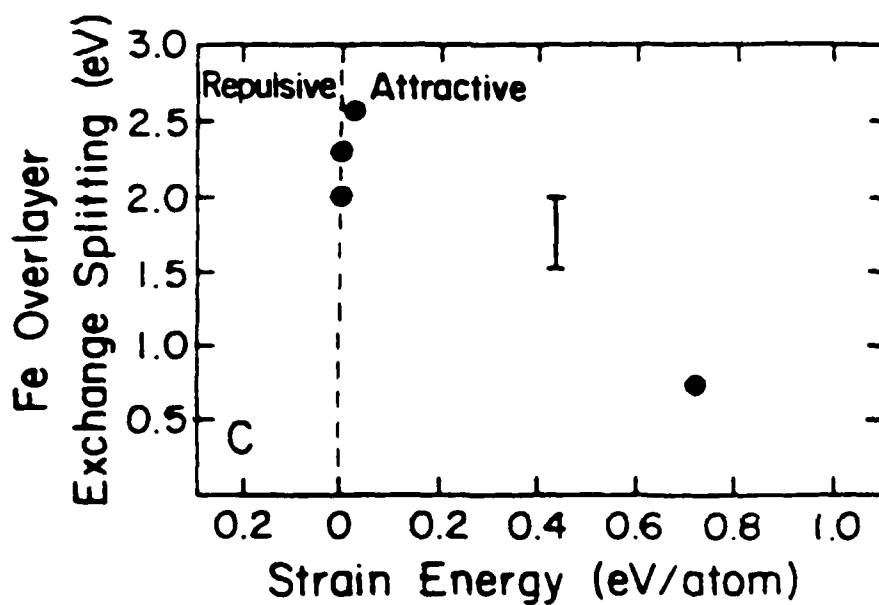
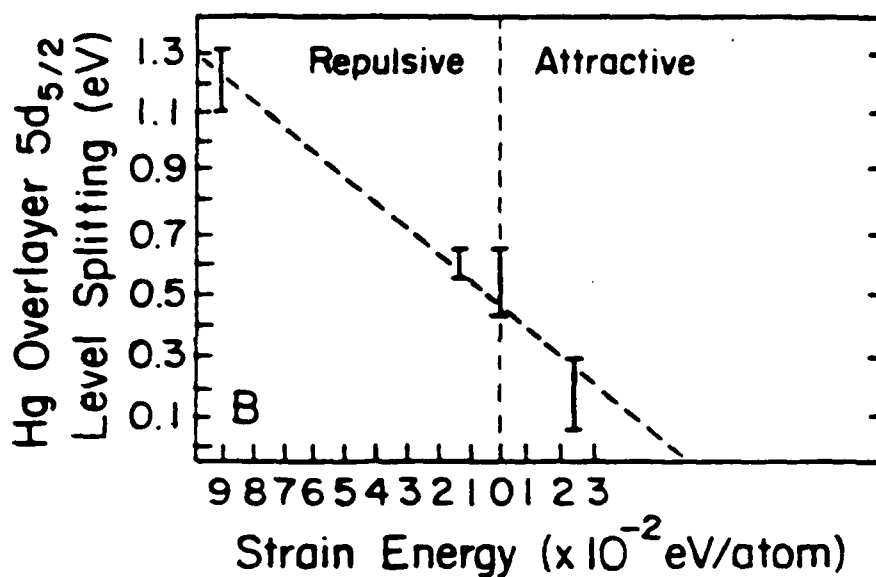
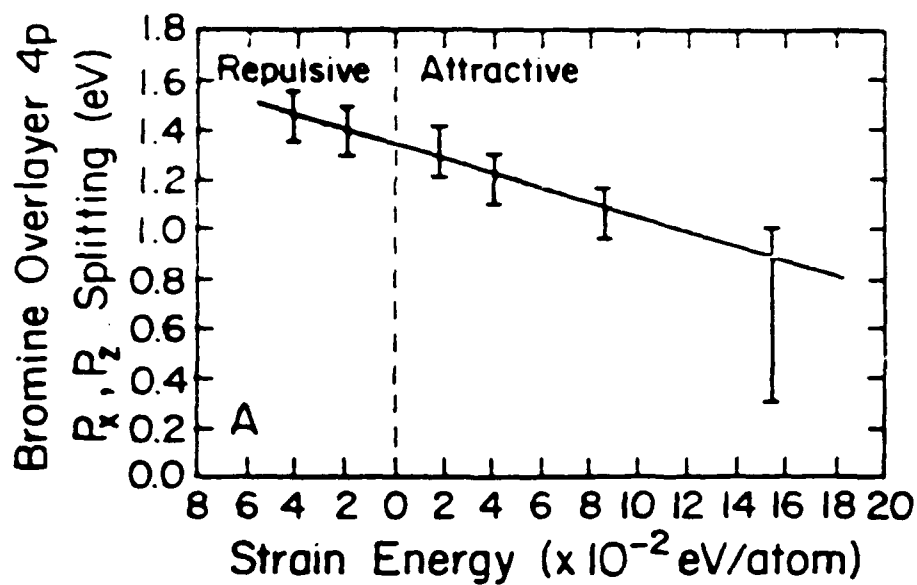


Figure 1. The geometry of angle resolved photoemission indicating incidence angle θ_i , electron emission angle θ_e , and orientation angle of the electron wave vector with respect to the crystal ϕ . As is indicated in the figure the vector potential of the incident light has a perpendicular component and parallel component with respect to the surface as does the electron wave vector.

TECHNICAL PROGRESS

In the ten months of the project virtually all the goals were accomplished. By investigating model systems it has been possible to demonstrate that:

- 1) The work function of a complex surface cannot be ascertained by simply exploring the local chemistry and basing the work function upon the expected charge transfer between atoms expected as a result of the chemical bonding [1]. This was demonstrated by investigating the electronic structure of halogen overlayers, and using the observed experimental data in electrostatic calculations modeling the charge transfer to the surface [1]. These results should be generally applicable to other systems.
- 2) We have shown that the long range crystallographic order of a system has a substantial influence upon the electron structure and density of states of thin metal overlayers [2-4]. This means that the surface electronic properties (including work function) cannot be made independent of the crystallographic order.
- 3) Thin metal films can be strained, and the strain is directly proportional to the change in the valence band electron structure [5]. Thus by changing the lattice constant of a material, the electronic structure can be changed [5]. Increasing the thickness of a strained thin film will allow the film to relieve strain, but the change in the electronic structure is related to this strain relief in a complex manner [6]. These results relating strain to electronic structure are generally applicable to all metal overlayers, including the alkali metals [5]. These results are summarized in figure 2.



In the figure the separation of degenerate valence levels (lifted as a result of strain) are plotted against calculated strain energies, treating attractive and repulsive strain separately.

The investigations were centered on metal overlayer systems that would provide results in the short period of time allowed by the funding of the contract. Thus the systems investigated were Br/Fe, I/Fe, Hg/Ag, Hg/Cu, Hg/Cu₃Au, Fe/Cu, Fe/Ag, and Cs/W. None of these materials are particularly important components to field emitter cathodes, though the physics elucidated from the study of these systems is of particular value in understanding the physics of the field emitter cathode surface. Several problems remain and further research is indicated. First, the investigation of barium thin films is strongly indicated since this is both an ideal metal for investigating the electronic structure of thin metal overlayers and because barium is an important component of field emitter cathodes. Complete studies of barium were not possible due to the unavailability of time at the synchrotron and the short period covered by the contract. Secondly, the electronic structure, surface layer strain and the barium cluster size should be characterized for field emitter cathodes so that model calculations (employing the results of this project) can be undertaken. These calculations would be most valuable in understanding how the field emitter cathode works at the microscopic level. To undertake these further studies would require an additional commitment to this type of research.

In summary, this was a project that proved to be very successful as measured by the quality and quantity of the results that emerged from the research. For a very limited expenditure, there has been a considerable

improvement in our understanding of the physics of thin metal overlayers, and these results can be employed to model and understand the processes related to a number of technologies (field emitter cathodes, VLSI, and electronic structure of semiconductor devices in reduced dimensionality such as quantum wells).

Publications

- [1] P.A. Dowben, Y.J. Kime, D.R. Mueller, and T.N. Rhodin, J. Chem. Phys., 89 (1988) 4406.
- [2] M. Onellion, P.A. Dowben, and J.L. Erskine, Phys. Lett., A130 (1988) 171.
- [3] Shikha Varma, Y.J. Kime, D. LaGrafte, P.A. Dowben and M. Onellion, Z. Naturforsch., in press.
- [4] P.A. Dowben, M. Onellion, S. Varma, Y.J. Kime and J.L. Erskine, J. Vac. Sci. Technol., A7 (1989) 2070-2074.
- [5] P.A. Dowben, Shikha Varma, Y.J. Kime, D.R. Mueller, and M. Onellion, Zeitschrift fuer Physik B73 (1988) 247-255.
- [6] Shikha Varma, Y.J. Kime, P.A. Dowben and M. Onellion, Proc. Mat. Res. Soc. 143 (1989) 85-90.

Summary: 5 papers published, one paper submitted for publication as of 10/88. All papers are appearing in refereed journals of the highest quality. In addition to these papers, there are also two published abstracts resulting from this work. They are:

- [1] Shikha Varma, Y.J. Kime, P.A. Dowben, and M. Onellion, Bull. Am. Phys. Soc. 33 (1988) 562.
- [2] Y.J. Kime, P.A. Dowben, D. Mueller and T.N. Rhodin, Bull. Am. Phys. Soc., 33 (1988) 737.



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